

Magnetic and High-Pressure Effects on the Elastic and Structural Properties of Iron

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Assuming saturated ferromagnetism, the anomalous crystal structures and elastic constants of the magnetic 3d transition metals Fe, Co, and Ni can be explained by simple band-filling arguments.¹ The exceptional elastic properties of bcc Fe are well described by *ab initio* FP-LMTO electronic structure calculations using the local spin-density approximation. The behavior of the tetragonal shear constant C' can be understood from the d -band filling of the minority spin band, while the almost filled majority spin-band contribution can be neglected. This configuration of 3d band electrons in ferromagnetic metals explains their anomalously low elastic constants as well as their crystal structures. At reduced volumes, we are examining the elastic and structural properties of nonmagnetic Fe, whose high-pressure phase diagram is of current geophysical interest. Possible metastable fcc and bct structures have been identified in addition to the stable hcp structure. Our goal here is to use calculated elastic, structural, and vibrational data to develop accurate many-body interatomic potentials with which both high-temperature phase stability and melting can be addressed.

¹P. Söderlind, et. al, Phys. Rev. B **50**, 5918 (1994).

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